

FIG. 1

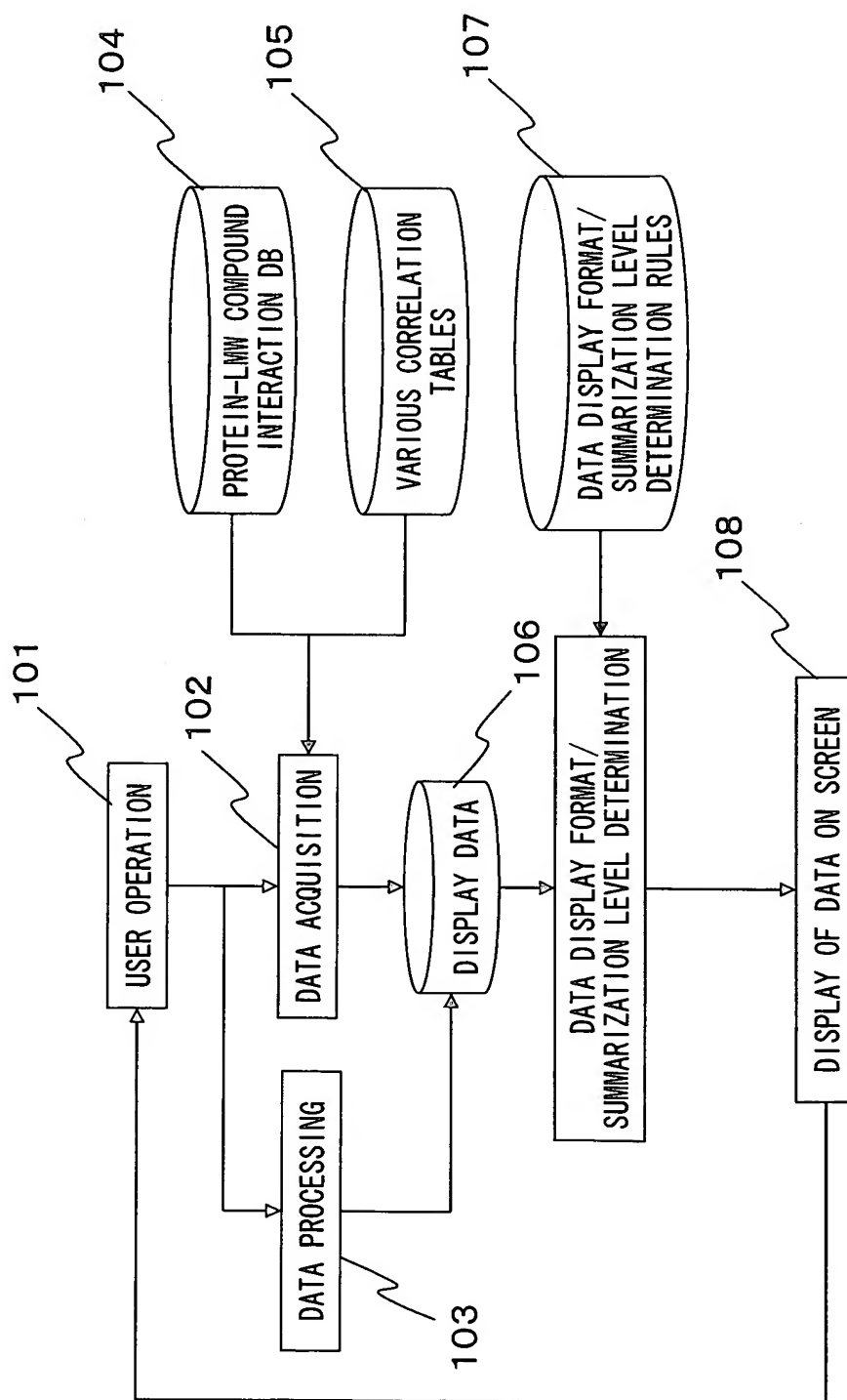


FIG. 2

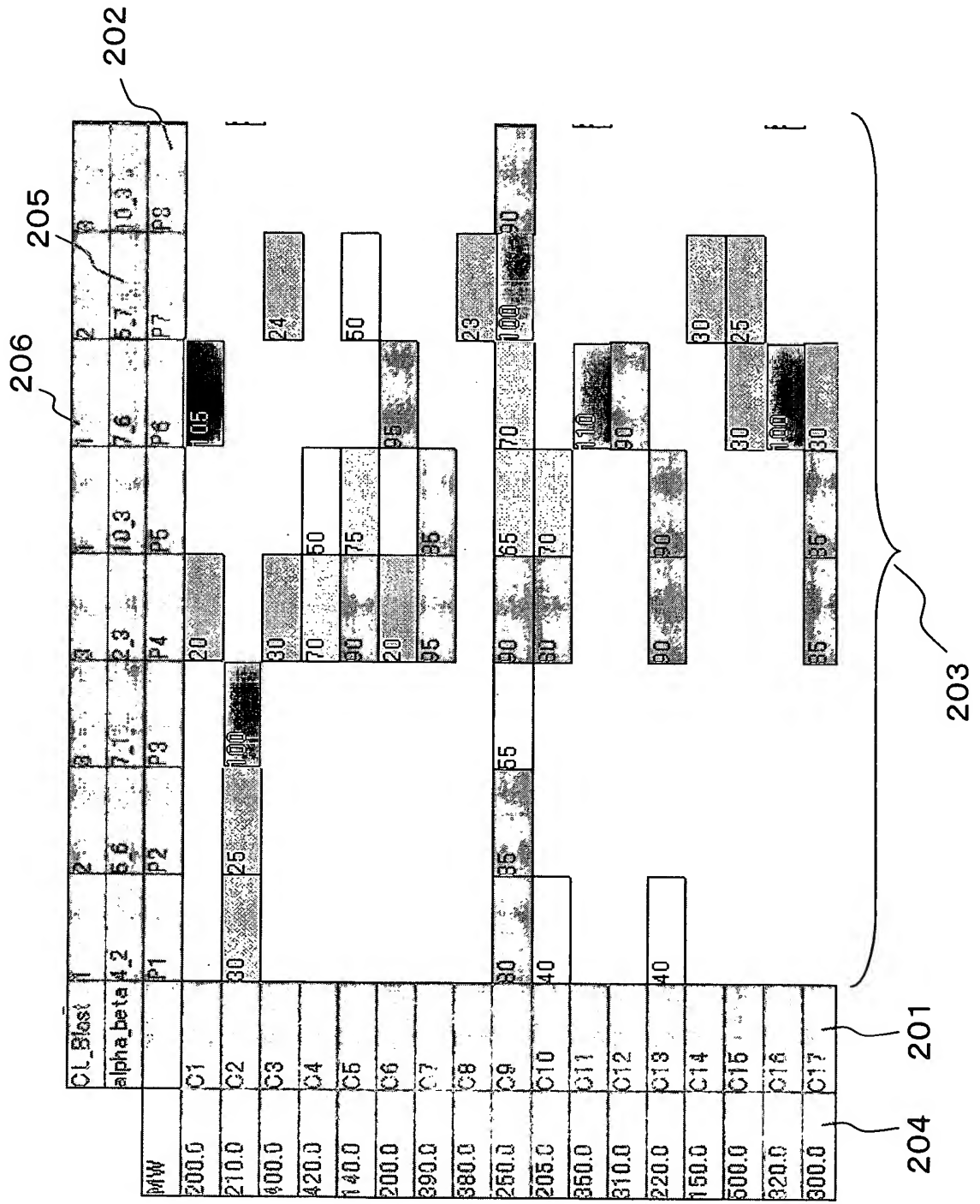


FIG. 3

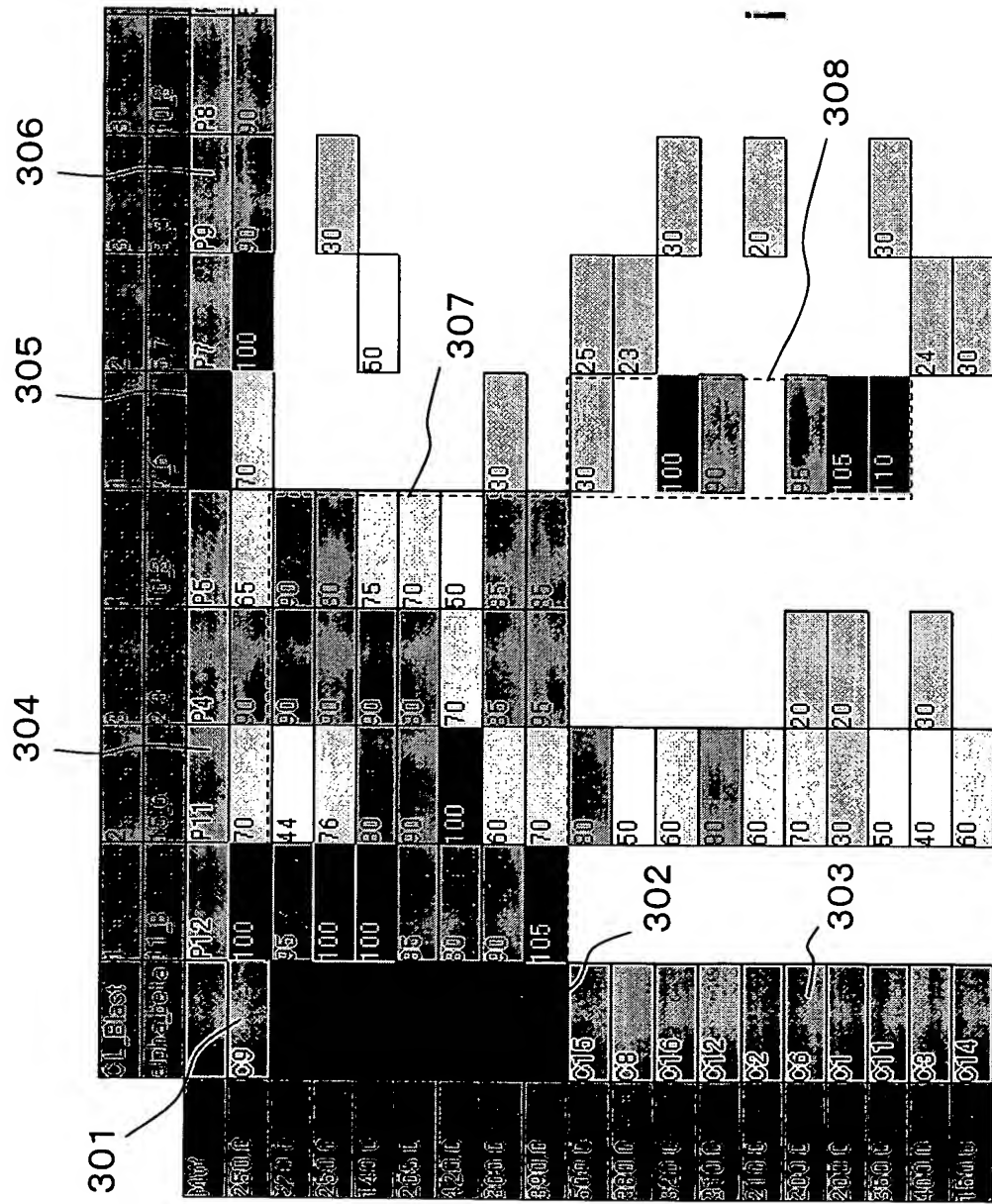


FIG. 4

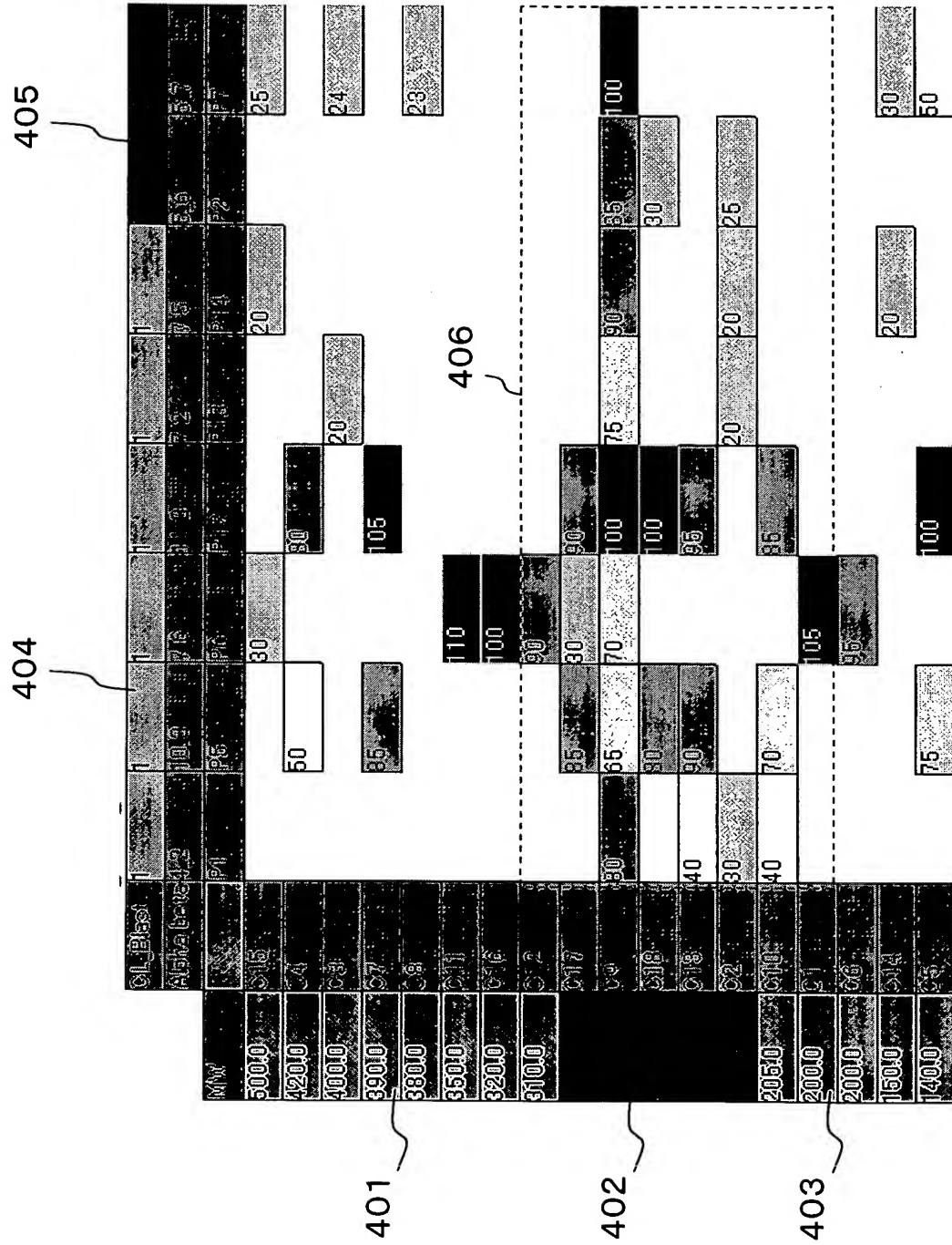


FIG. 5

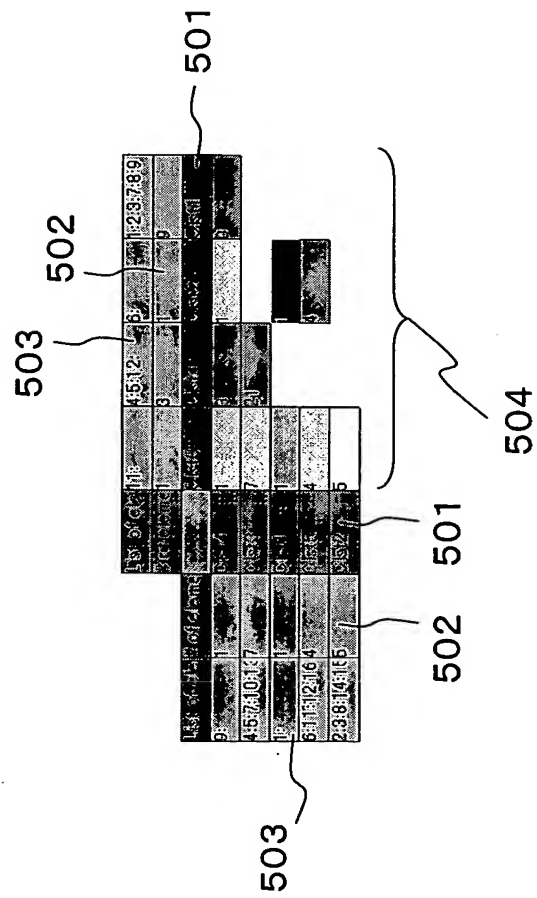


FIG. 6

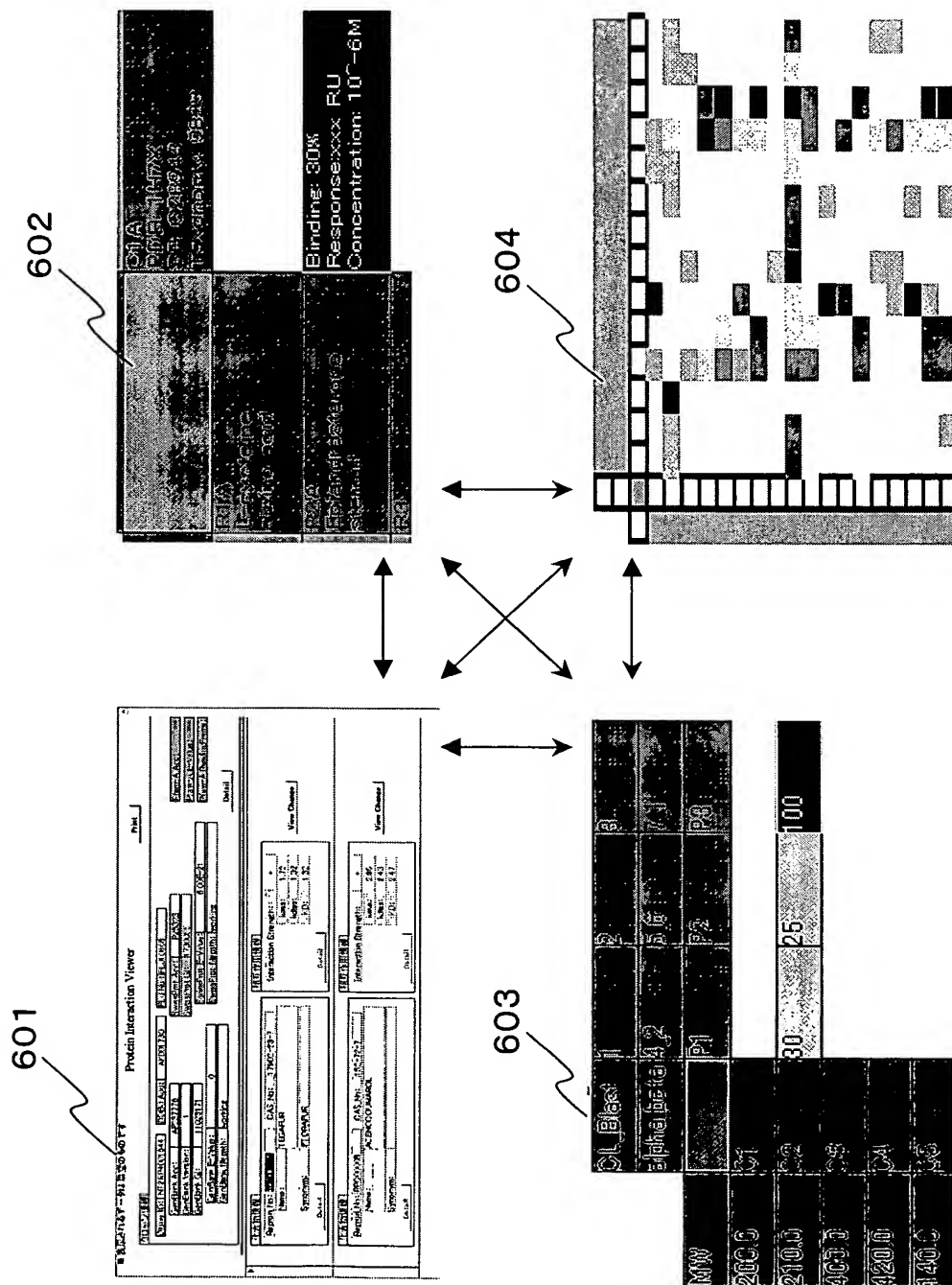


FIG. 7

SUMMARIZATION/ LEVEL	DATA ITEM	LOCATION	SUMMARIZATION RULE
1	NAME OF COMPOUND	LABEL	AS IS
1	MOLECULAR WEIGHT	FEATURE QUANTITY DESCRIPTION CELL	AS IS
1	PHYSICAL PROPERTY CLUSTER NUMBER	FEATURE QUANTITY DESCRIPTION CELL	AS IS
1	NAME OF DRUG EFFICACY CLUSTER	FEATURE QUANTITY DESCRIPTION CELL	AS IS
2	COMPOUND ID	LABEL	LAST 5 DIGITS
2	MOLECULAR WEIGHT	FEATURE QUANTITY DESCRIPTION CELL	ROUND TO WHOLE NUMBER
2	PHYSICAL PROPERTY CLUSTER NUMBER	FEATURE QUANTITY DESCRIPTION CELL	LAST 5 DIGITS
2	DRUG EFFICACY CLUSTER NUMBER	FEATURE QUANTITY DESCRIPTION CELL	LAST 5 DIGITS
2	NAME OF DRUG EFFICACY CLUSTER	INFORMATION DISPLAY SEPARATE SCREEN	LINK FROM DRUG EFFICACY CLUSTER NUMBER; AS IS
3	COMPOUND ID	INFORMATION DISPLAY SEPARATE SCREEN	LINK FROM LABEL; AS IS
3	MOLECULAR WEIGHT	FEATURE QUANTITY DESCRIPTION CELL	COLORS (200, 300, 400, 500)
3	PHYSICAL PROPERTY CLUSTER NUMBER	FEATURE QUANTITY DESCRIPTION CELL	COLORS (DIFFERENT COLOR FOR EACH NUMBER)
3	NAME OF DRUG EFFICACY CLUSTER	FEATURE QUANTITY DESCRIPTION CELL	COLORS (DIFFERENT COLOR FOR EACH NUMBER)

FIG. 8

801		802		803
CONDITION		DISPLAY FORMAT	SUMMARIZATION LEVEL	
$P \times C \leq 3$		INDIVIDUAL DATA DISPLAY	0	
$G \leq 11 \text{ \& } R \leq 11$		INDIVIDUAL DATA DISPLAY	1	
$G \leq 34 \text{ \& } R \leq 22$		INDIVIDUAL DATA DISPLAY	2	
$G \leq 135 \text{ \& } R \leq 270$		INDIVIDUAL DATA DISPLAY	3	
$G_c \leq 11 \text{ \& } R_c \leq 11$		CLUSTER DISPLAY	1	
$G_c \leq 34 \text{ \& } R_c \leq 22$		CLUSTER DISPLAY	2	
$G_c \leq 135 \text{ \& } R_c \leq 270$		CLUSTER DISPLAY	3	
OTHERS		STATISTICAL DISPLAY	0	
DEFINITION		G: P + NUMBER OF DISPLAYS OF PHYSICAL PROPERTY IN COLUMN DIRECTION + 1 R: C + NUMBER OF DISPLAYS OF PHYSICAL PROPERTY IN COLUMN DIRECTION + 1 Gc: Pc + NUMBER OF DISPLAYS OF PHYSICAL PROPERTY IN COLUMN DIRECTION + 1 Rc: Cc + NUMBER OF DISPLAYS OF PHYSICAL PROPERTY IN COLUMN DIRECTION + 1		



COMPOUND/ COMPOUND	C1	C5	C9	C7
C1		☆		☆
C5	☆		☆	
C9	☆	☆		
C7	☆	☆		☆

COMPOUND/ PROTEIN	P1	P5	P12	P14	P16
C1					
C5					
C9					
C7					

PROTEIN/ PROTEIN	P1	P5	P12	P14	P16
P1		90		100	
P5	100			100	
P12		75		45	50
P14	100	70			

EXPRESSION /PROTEIN	P1	P5	P12	P4	P16
G3	+			+	
G4		++			-
G8	++	-	+		++
G1				+	

FIG. 10

RELATED INFORMATION ABOUT (R5, C12), (R9, C12)  
FROM PROTEIN-EXPRESSION TABLE:      xx ITEMS  
FROM PROTEIN-PROTEIN INTERACTION TABLE:      yy ITEMS  
FROM LMW COMPOUND-LMW COMPOUND INTERACTION TABLE:      zz ITEMS

FIG. 11

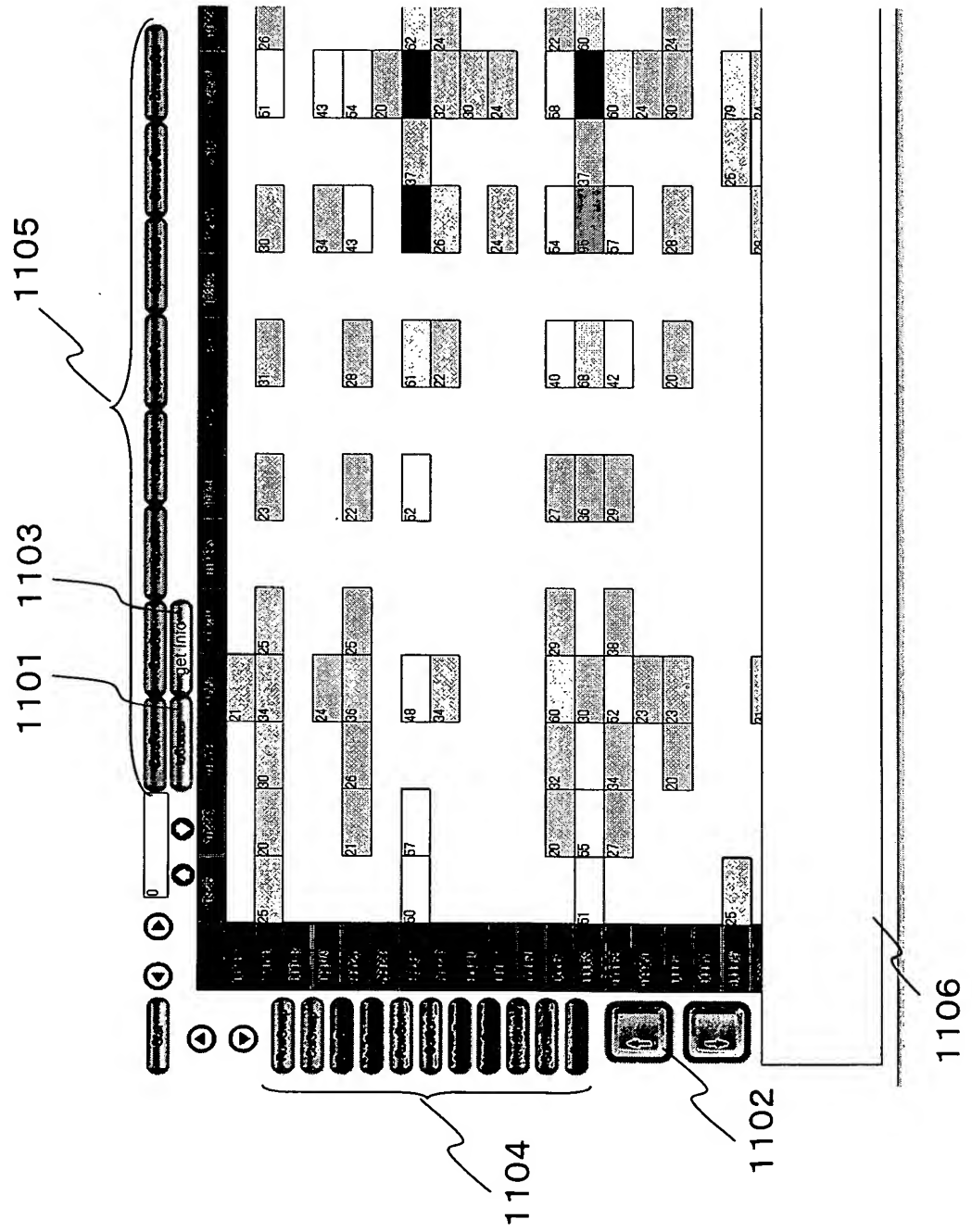


FIG. 12 A

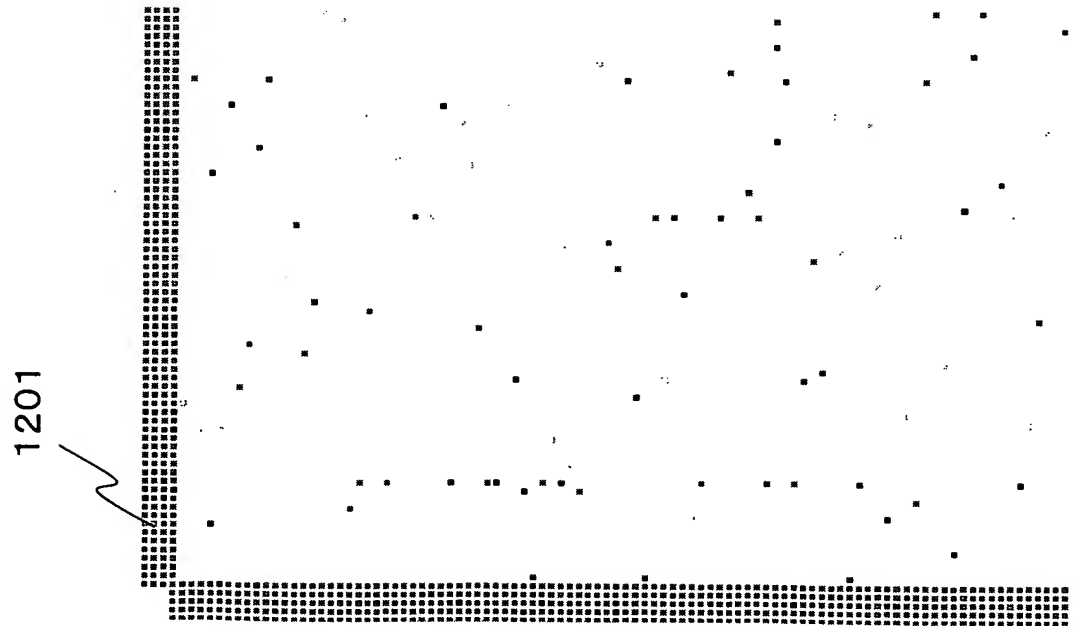


FIG. 12 B

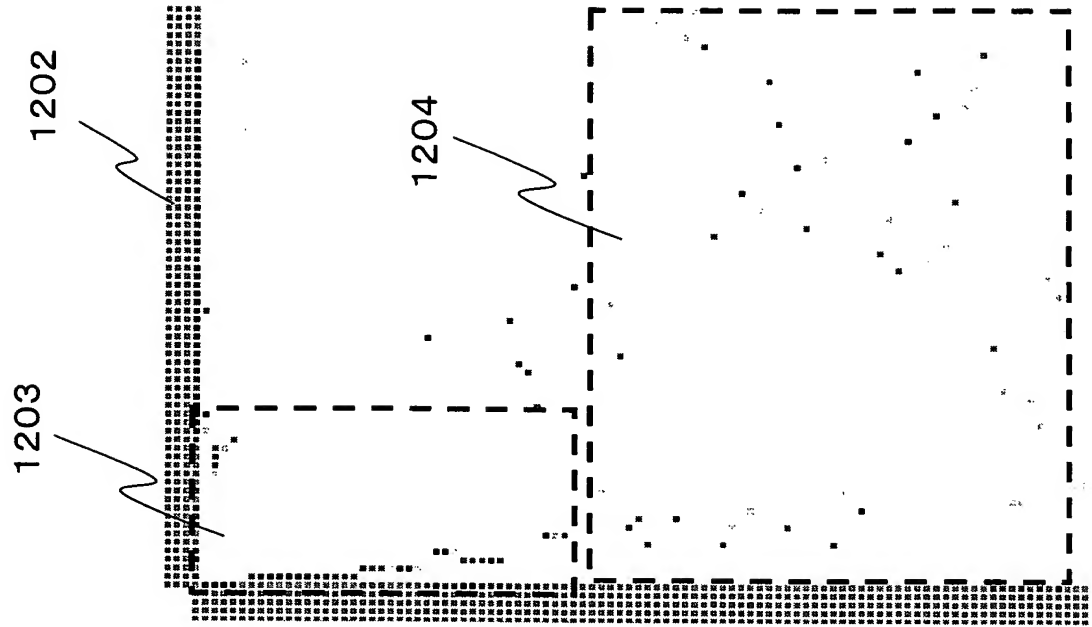


FIG. 13 A

Members #	Cist	Members #	Cist	Members #	Cist	Members #	Cist
20:23:30:12	Cist12	43:1	Cist10	56:1	Cist12	59:1	Cist15
26:28:52:17	Cist17	7:1	Cist11	7:1	Cist11	7:1	Cist11
6:29:36:3	Cist5						
2:10:49:6:5	Cist2						
16:82:87:3	Cist14						
22:79:2	Cist19						
35:2	Cist3						
18:65:2	Cist25						
1:31:32:3:44	Cist11						

FIG. 13 C

LogP	MR	NAME OF COMPOUND	BINDING
INTERMEDIATE	SMALL	AE2	WEAK
<u>SMALL</u>	<u>INTERMEDIATE</u>	STR	STRONG
<u>SMALL</u>	<u>LARGE</u>	SIH	STRONG
<u>LARGE</u>	<u>LARGE</u>	S5H	INTERMEDIATE
<u>SMALL</u>	SMALL	ANO	INTERMEDIATE

FIG. 13 B

LOGP	QMR	MW	CLASS	LOGP	QMR	MW	CLASS
0.046999	9.023698	890.461	HETEROCALB	1.00E-10	3.10	200	CATH
13.425	20.18835	649.1010	HETEROCAL4	3.24E-10	42.11	277	FC
5.179999	9.628871	304.474	HETEROCETS	3.72E-10	277	493	52118
1.0257	6.608605	296.392	HETEROCETS	1.51E-09	200918	NA	NA
1.572	21.67711	804.0310	HETEROCAL5	1.29E-10	Carbonic	HIV-1	pc
0.268000	7.119789	810.4190	HETEROCAL5	4.57E-10	FK506	bin	F357
-1.323	3.558921	151.129	HETEROCAL3	2.00E-10	NA	NA	NA
6.874000	24.87121	914.1869	HETEROCAL3	1.00E-10	NA	NA	NA
1.155	9.693314	849.431	HETEROCAL7	1.00E-10	NA	NA	NA
1.397	15.68304	677.7229	HETEROCAL2	1.58E-10	NA	NA	NA
4.345769	10.77762	407.604	HETEROCAL2	1.56E-09	NA	NA	NA
0.234	12.44736	175.465	HETEROCAL9	4.90E-10	NA	NA	NA
0.745	8.902669	374.4620	PEPTIDOGAN	1.27E-07	NA	NA	NA
-99.9	-1	-1	NA	6.28E-14	NA	NA	NA
-99.9	-1	-1	NA	7.74E-13	NA	NA	NA
4.642000	21.63643	751.948	STANDAF337	2.04E-10	NA	NA	NA
-99.9	-1	-1	NA	7.05E-09	NA	NA	NA
-99.9	-1	-1	NA	7.79E-07	NA	NA	NA
0.386999	9.681050	403.604	PEPTIDICPSI	2.80E-09	NA	NA	NA
1.248	8.650813	362.4509	HETEROCBS3	3.46E-07	NA	NA	NA
2.778999	16.56522	685.7899	RINGSWIRAP	2.00E-10	NA	NA	NA
0.880999	8.841756	372.4460	RINGSWIRK5	1.97E-10	NA	NA	NA
3.622999	8.348864	290.4489	AND M(AE2	9.87E-10	NA	NA	NA
3.301000	9.178498	614.4689	AND M(STR	3.57E-10	NA	NA	NA
2.430000	11.55415	430.5409	NA	2.00E-09	NA	NA	NA
4.577000	11.49878	418.5740	AND M(S5H	7.98E-09	NA	NA	NA
3.043	8.312344	288.431	3 AND M(ANO	2.00E-09	NA	NA	NA
-6.07393	14.82128	667.4859	STANDAFOL	1.97E-10	NA	NA	NA
0.609000	7.559960	324.4460	STANDAFMTX	2.69E-06	NA	NA	NA
-2.00046	5.577835	237.2189	HETEROCBIO		NA	NA	NA

FIG. 14 A

	P1	P2	P3	P4	P5	P6	P7
T1		●				●	●
T2				●	●		
T3			●	●	●		
T4				●	●	●	●
T5						●	●
T6	●			●	●		
T7			●				

1402 1410 1411

FIG. 14 B

	S1	S2	S3	S4	S5
C1	●				
C2		●	●		
C3		●	●		
C4		●	●	●	●
C5		●	●	●	●
C6			●		

1403 1412 1413

FIG. 14 C

	P1	P2	P3	P4	P5	P6	P7
C1							
C2							
C3							
C4							
C5							
C6							

1401 1408 1409 1405 1404 1406 1407

FIG. 15

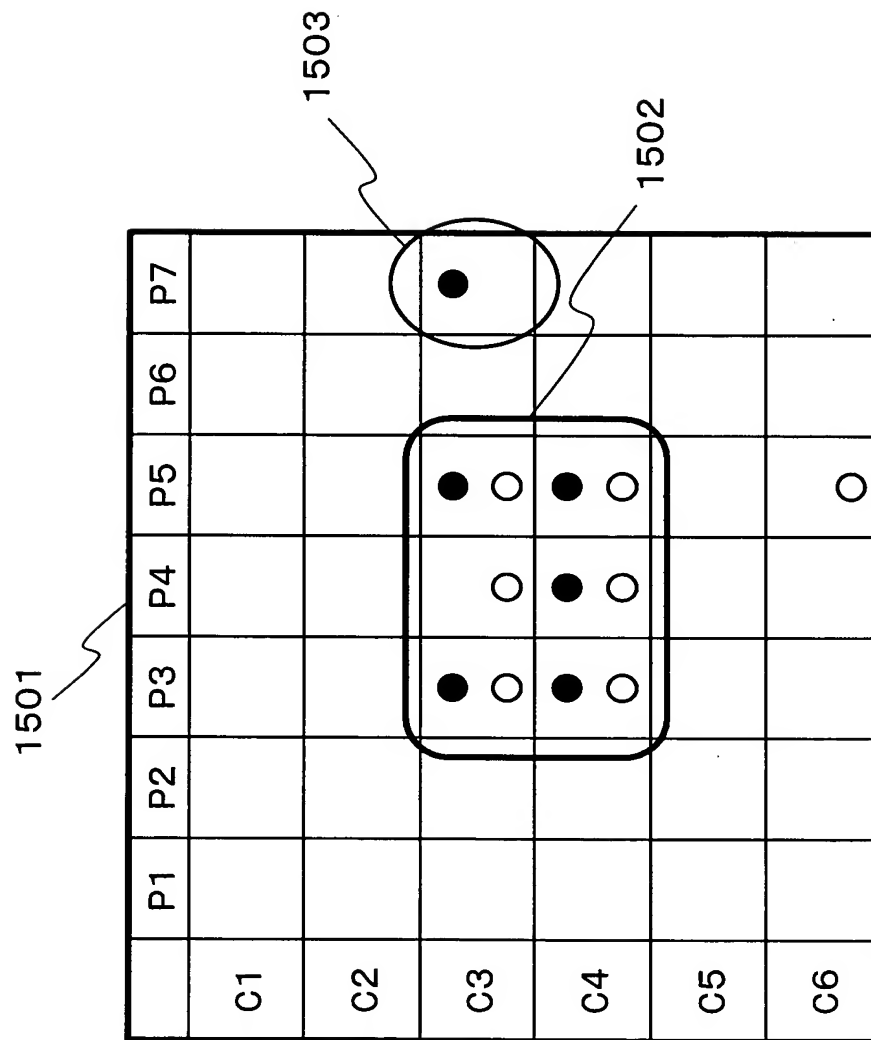


FIG. 16

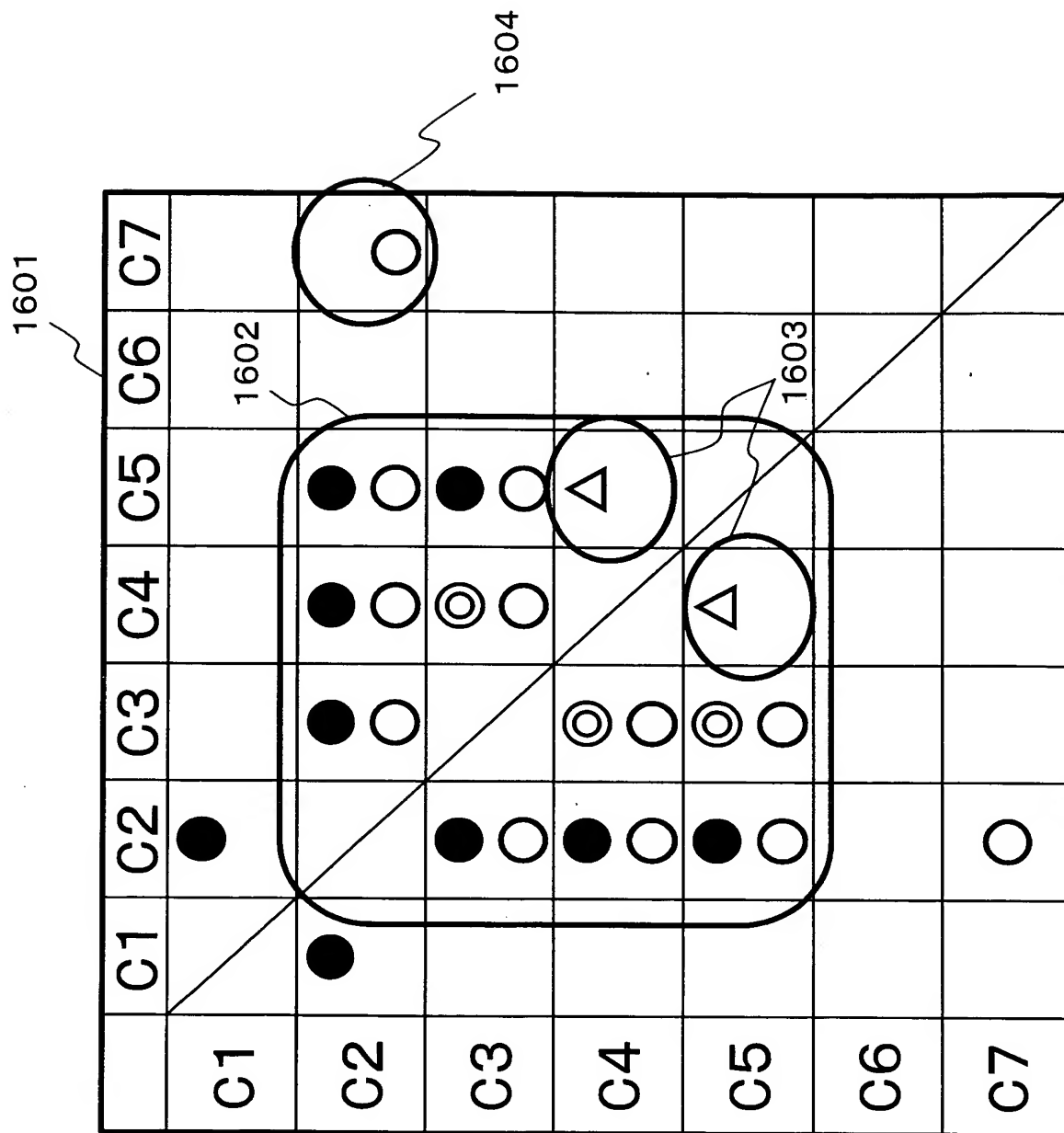




FIG. 17 A

1701

	R3	R2	R4	R1	R5	C1	R6	R7	R9	R8
R3		●	●							
R2	●			●						
R4	●			●	●					
R1		●	●	●	●	●	●	●	●	●
R5			●	●	●	●	●	●	●	●
C1				●	●	●	●	●	●	●
R6					●	●	●	●	●	●
R7							●	●	●	●
R9								●	●	●
R8								●	●	●

1702

FIG. 17 B

